MAS15-2015-000017

Abstract for an Invited Paper for the MAS15 Meeting of the American Physical Society

Electron correlations in solids from the Dynamical Mean Field perspective and the origin of the anomalous state of matter in iron pnictides and chalchogenides KRISTJAN HAULE, Rutgers Univ

Materials with strong electronic correlations have long resisted abinitio modeling due to their complexity arising from nonperturbative strength of the interaction. The Dynamical Mean Field Theory in combination with the Density Functional Theory has recently changed that, and enabled detailed modeling of the electronic structure of many complex materials, such as the heavy fermions, transition metal oxides, iron superconductors. I will give basic foundation of this theory from the functional point of view, and an overview on the recent advances in this field. As an example, I will discuss the iron superconductors and their anomalous properties, which have their origin in strong Hund's coupling and give rise to physics of Hund's metals. The Dynamical Mean Field Theory simulations not only uncovered the origin of the anomalous properties, but also successfully explained the key properties of these material: such as the mass renormalizations and anisotropy of quasiparticles, the crossover into an incoherent regime above a low temperature scale, and the magnetic excitations in energy and momentum space, the spin dynamics and superconducting pairing symmetry. A novel orbital anti-phase superconducting pairing was discovered, which explains the measured gaps on Fermi surfaces.